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TERMINAL (ENTER 1, 2, 3, OR ?):2

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* * * * * *
                    Welcome to STN International
                Web Page for STN Seminar Schedule - N. America
NEWS
NEWS
     2 MAY 01 New CAS web site launched
NEWS 3 MAY 08
                CA/CAplus Indian patent publication number format defined
NEWS 4 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display
NEWS 5 MAY 21 BIOSIS reloaded and enhanced with archival data
NEWS 6 MAY 21
                TOXCENTER enhanced with BIOSIS reload
NEWS 7 MAY 21
                CA/CAplus enhanced with additional kind codes for German
                patents
NEWS 8 MAY 22
                CA/CAplus enhanced with IPC reclassification in Japanese
                patents
NEWS 9
        JUN 27
                CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10
        JUN 29 STN Viewer now available
NEWS 11 JUN 29
                STN Express, Version 8.2, now available
NEWS 12 JUL 02 LEMBASE coverage updated
NEWS 13 JUL 02 LMEDLINE coverage updated
NEWS 14 JUL 02 SCISEARCH enhanced with complete author names
NEWS 15 JUL 02 CHEMCATS accession numbers revised
                CA/CAplus enhanced with utility model patents from China
NEWS 16 JUL 02
NEWS 17 JUL 16 CAplus enhanced with French and German abstracts
NEWS 18 JUL 18 CA/CAplus patent coverage enhanced
NEWS 19 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20 JUL 30 USGENE now available on STN
NEWS 21 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 22 AUG 06 BEILSTEIN updated with new compounds
NEWS 23 AUG 06 FSTA enhanced with new thesaurus edition
NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
             CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
             AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.
NEWS HOURS
             STN Operating Hours Plus Help Desk Availability
             Welcome Banner and News Items
NEWS LOGIN
NEWS IPC8
             For general information regarding STN implementation of IPC 8
```

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

E

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:26:41 ON 06 AUG 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES:

5 AUG 2007 HIGHEST RN 944042-79-9

DICTIONARY FILE UPDATES:

5 AUG 2007 HIGHEST RN 944042-79-9

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10-552504.str

#### L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1

STR

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 14:28:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED 1636 ITERATIONS

17 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

30294 TO 35146

PROJECTED ANSWERS:

93 TO 587

L2

17 SEA SSS SAM L1

=> d scan

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-

hydroxyphenyl) -, (2R, 3aR, 4S, 9bS) - (9CI)

MF C18 H17 F O3

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benz[b] indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI)

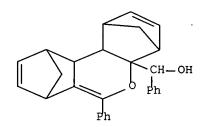
MF C34 H24 O

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro- $\alpha$ ,6-diphenyl-, [1 $\alpha$ ,4 $\alpha$ ,4a $\beta$ (R\*),7 $\beta$ ,10. beta.,10a $\alpha$ ,10b $\beta$ ]- (9CI)

MF C28 H26 O2



### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI)

MF C32 H30 O4

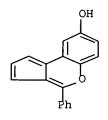
Relative stereochemistry.

# HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI)

C18 H12 O2 MF



# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

# HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI)

MF C32 H26 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9bhexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI)

MF C19 H16 F2 O3

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[d] naphtho[1,2-b] pyran-11-ol, 6-phenyl- (9CI)

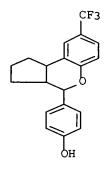
MF C22 H14 O2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benz opyran-4-yl]- (9CI)

MF C19 H17 F3 O2



### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Silane, (1,1-dimethylethyl) [4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-

, rel- (9CI) MF C35 H54 O3 Si3

Relative stereochemistry.

PAGE 2-A

Me Me

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

Uploading C:\Program Files\Stnexp\Queries\10-552504a.str

### L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3

STR

Structure attributes must be viewed using STN Express query preparation.

=> s 13 sss sam

SAMPLE SEARCH INITIATED 14:43:40 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2835 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

53507 TO 59893

PROJECTED ANSWERS:

O TO

0 SEA SSS SAM L3

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

13.95 14.16

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=> s 12 and (py<2004 or ay<2004 or pry<2004)

8 L2

23927525 PY<2004

4731037 AY<2004

4212934 PRY<2004

6 L2 AND (PY<2004 OR AY<2004 OR PRY<2004) L5

=> d scan

6 ANSWERS L5 CAPLUS COPYRIGHT 2007 ACS on STN

IC ICM C07D311-00

```
27-7 (Heterocyclic Compounds (One Hetero Atom))
CC
     Section cross-reference(s): 1, 63
ΤI
   Preparation of substituted benzopyrans as selective estrogen receptor-beta
     agonists
ST
     benzopyran prepn estrogen receptor beta agonist anticancer
IT
     Prostate gland, disease
        (benign hyperplasia; preparation of cyclopenta[c]chromenols as selective
        estrogen receptor-beta agonists)
IT
     Hyperplasia
        (benign prostatic; preparation of cyclopenta[c]chromenols as selective
        estrogen receptor-beta agonists)
IT
     Prostate gland, neoplasm
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
        agonists)
IT
     Antitumor agents
        (prostate gland; preparation of cyclopenta[c]chromenols as selective
        estrogen receptor-beta agonists)
IT
     Estrogen receptors
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (β; preparation of cyclopenta[c]chromenols as selective estrogen
        receptor-beta agonists)
IT
     787621-59-4P
                    787621-60-7P
                                   787621-80-1P 787621-81-2P
     787622-06-4P
                    787622-10-0P
                                   787622-73-5P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
        agonists)
IT
     787621-53-8P
                    787621-54-9P
                                   787621-55-0P
                                                  787621-56-1P
                                                                 787621-57-2P
     787621-58-3P
                    787621-61-8P
                                   787621-62-9P
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                                                  787621-63-0P
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                                   787621-73-2P
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     787622-85-9P
                    787622-86-0P
                                   787622-87-1P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
        agonists)
IT
    62-23-7, p-Nitrobenzoic acid
                                    75-86-5, Acetone cyanohydrin
    Methyl acrylate
                     96-35-5, Methyl glycolate
                                                   100-39-0, Benzyl bromide
     123-31-9, Hydroquinone, reactions
                                         623-82-5, (R) - (+) -3-Methyladipic acid
     892-20-6, Triphenyltin hydride
                                    1066-54-2, Trimethylsilylacetylene
    1100-88-5, Benzyltriphenylphosphonium chloride
                                                      1530-32-1,
    Ethyltriphenylphosphonium bromide
                                        2365-48-2, Methyl thioglycolate
    2622-05-1, Allylmagnesium chloride 3058-01-3, 3-Methyladipic acid
    5781-53-3, Methyl chloroglyoxylate
                                          6228-47-3, Propyltriphenylphosphonium
              6793-92-6, p-Benzyloxybromobenzene
                                                    10347-88-3,
     3-tert-Butyladipic acid 10538-51-9, 2,5-Dimethoxycinnamic acid
```

```
22444-89-9, Butyltriphenylphosphonium 25458-45-1, 1-Bromo-4-
     (methoxymethoxy) benzene 37595-74-7, N-Phenyltrifluoromethanesulfonimide
     38053-91-7, 2-[(Trimethylsilyl)oxy]butadiene
                                                   38078-09-0,
     N,N-Diethylaminosulfur trifluoride 70160-51-9
                                                      72047-94-0,
     [2-(Acetoxymethyl)allyl]trimethylsilane
                                              108270-19-5
                                                            146631-00-7.
     4-(Benzyloxy)phenylboronic acid
                                     787622-05-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
        agonists)
IT
     2689-68-1P
                  4463-74-5P
                              6093-68-1P, 6-Hydroxycoumarin
                                                              57595-23-0P
     87905-74-6P, 1,4-Bis (methoxymethoxy) benzene
                                                  608536-53-4P,
     6-Methoxymethoxycoumarin
                              787621-46-9P 787621-47-0P
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     787621-49-2P
                   787621-50-5P
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                   787622-19-9P 787622-20-2P 787622-21-3P 787622-23-5P,
     6-Benzyloxychromen-2-one 787622-25-7P 787622-26-8P
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                                                                787622-67-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
        agonists)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
L5
      6 ANSWERS
                 CAPLUS COPYRIGHT 2007 ACS on STN
CC.
     10 (Organic Chemistry)
     Condensation of tetraphenylbutynediol with phenol
ΤI
IT
     Catalysts
        (for condensation, of PhOH with 1,1,4,4-tetraphenyl-2-butyne-1,4-diol)
     411220-98-9P, Indene, 1-benzohydrylidene-2-chloro-3-phenyl-
IT
     411220-98-9P, Methane, (2-chloro-3-phenyl-1-indenylidene)diphenyl-
     854748-48-4P, Methane, [2-(p-methoxyphenyl)-3-phenyl-1-
     indenylidene]diphenyl- 854748-48-4P, Anisole, p-(1-benzohydrylidene-3-
     phenyl-2-indenyl) - 854748-48-4P, Indene, 1-benzohydrylidene-2-(p-
     methoxyphenyl) - 3-phenyl - 854749-76-1P, Indene, 1-benzohydrylidene-2-
     phenoxy-3-phenyl- 854749-76-1P, Methane, (2-phenoxy-3-phenyl-1-
     indenylidene)diphenyl- 860000-10-8P, Furan, 2,5-dihydro-3-phenoxy-
     2,2,5,5-tetraphenyl- 860186-11-4P, Benz[b]indeno[2,1-d]pyran,
     6,6a-dihydro-6,6,11-triphenyl- 861008-63-1P, Phenol,
    p-(1-benzohydrylidene-3-phenyl-2-indenyl)-
     RL: PREP (Preparation)
        (preparation of)
IT
     1483-74-5, 2-Butyne-1,4-diol, tetraphenyl-
        (reaction with phenol)
IT
     108-95-2, Phenol
        (reactions of, with 1,1,4,4-tetraphenyl-2-butyne-1,4-diol)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0
=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y
L5
    ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
```

ACCESSION NUMBER:

2004:927190 CAPLUS Full-text

DOCUMENT NUMBER:

141:395410

TITLE:

Preparation of substituted benzopyrans as selective

estrogen receptor-beta agonists

INVENTOR(S):

Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer,

Lance Allen; Richardson, Timothy Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE --------------------WO 2004094400 20041104 WO 2004-US9272 A2 20040408 <--WO 2004094400 Α3 20050224 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2004232798 **A1** 20041104 AU 2004-232798 20040408 <--CA 2518819 A1 20041104 CA 2004-2518819 20040408 <--EP 1626974 A2 20060222 EP 2004-759767 20040408 <--R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK BR 2004009588 20060418 Α BR 2004-9588 20040408 <--CN 1777614 Α 20060524 CN 2004-80010817 20040408 <--JP 2006524240 Т 20061026 JP 2006-509332 20040408 <--US 2007106082 Α1 20070510 US 2005-552504 20051006 <--

MX 2005-PA11243

US 2003-464404P

WO 2004-US9272

20051019 <--

P 20030421 <--

W 20040408

OTHER SOURCE(S):

MX 2005PA11243

PRIORITY APPLN. INFO.:

MARPAT 141:395410

20051215

Α

GI

$$HO$$
 $OH$ 
 $I$ 
 $Me$ 

Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multistep synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER- $\alpha$  subtype in the range 5.0 - >10,000 nM and to the ER- $\beta$  subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT 787621-81-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-88-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787621-99-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 787622-40-6 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RN 787622-43-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-78-0 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

#### IT 787622-29-1P 787622-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787622-29-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-41-7 CAPLUS

CN Silane, (1,1-dimethylethyl) [4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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L5 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2003:417738 CAPLUS Full-text

DOCUMENT NUMBER:

139:6768

TITLE:

Preparation of benzopyran derivatives as selective

estrogen receptor  $\beta$  agonists

INVENTOR(S):

Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar, Charles Willis, III; Neubauer, Blake Lee; Norman,

Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy

Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 138 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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	2003044					WO 2002-US33622	20021107 <				
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	RW: G	I, GM,	KE,	LS,	MW, MZ, SD,	SL, SZ, TZ, UG, ZM,	ZW, AM, AZ, BY,				
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EP	1448544	Į.		B1	20070516						
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JP	2005513	3027		T	20050512	JP 2003-545643	20021107 <				
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EP	1790644	Į.		A1	20070530	EP 2007-102693	20021107 <				
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AΤ	362471			Т	20070615	AT 2002-793806	20021107 <				
US	2004249				20041209	US 2004-493092	20040420 <				
US	7217734	<u> </u>		B2	20070515						
ZA	2004003	3733		Α	20051004	ZA 2004-3733	20040514 <				
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ORIT	Y APPLN	INFO	.:			US 2001-332766P	P 20011119 <				
						US 2002-363622P	P 20020311 <				
						EP 2002-793806	A3 20021107 <				

MARPAT 139:6768

AB The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor  $\beta$ agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor  $\beta$  (ER  $\beta$ ) with a Ki of <1 nM and Ki(ER  $\alpha$ )/Ki(ER  $\beta$ ) of 8.0. IT 533884-11-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor  $\beta$  agonists)

RN533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benz opyran-4-yl]- (9CI) (CA INDEX NAME)

5

L5 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1998:689997 CAPLUS Full-text

DOCUMENT NUMBER:

130:38272

TITLE:

A novel tandem bicyclization to form an indenopyran

ring system

AUTHOR (S):

Chakraborty, Manisha; McConville, David B.; Saito, Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier,

Claire A.; Youngs, Wiley J.

CORPORATE SOURCE:

Dep. of Chemistry, University of Akron, Akron, OH,

44325-3601, USA

SOURCE:

Tetrahedron Letters (1998), 39(45),

8237-8340

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been observed to give a highly conjugated ring system.

IT 216777-12-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of indenopyrans by tandem bicyclization)

RN 216777-12-7 CAPLUS

CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 6 ACCESSION NUMBER:

CAPLUS COPYRIGHT 2007 ACS on STN 1972:152831 CAPLUS Full-text

DOCUMENT NUMBER:

76:152831

TITLE:

Condensation of phenyl ethynyl ketone with

cyclopentadiene. Reinvestigation

AUTHOR (S):

Venkataramani, P. S.; Chandrasekharan, S.;

Swaminathan, S.

CORPORATE SOURCE:

Dep. Org. Chem., Univ. Madras, Madras, India

SOURCE:

Tetrahedron (1972), 28(5), 1249-55

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI For diagram(s), see printed CA Issue.

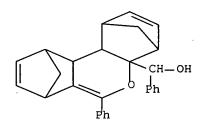
AB . The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(0)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT 36144-49-7P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

36144-49-7 CAPLUS RN

CN . 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10bhexahydro- $\alpha$ , 6-diphenyl-,  $[1\alpha, 4\alpha, 4a\beta(R^*), 7\beta, 10]$ . beta.,  $10a\alpha$ ,  $10b\beta$ ] - (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1969:77707 CAPLUS Full-text

DOCUMENT NUMBER:

70:77707

TITLE:

Experiments in the brazilane series. I. Preparation

of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S):

Morsingh, Francis

CORPORATE SOURCE:

Univ. Malaya, Kuala Lumpur, Malay. Tetrahedron (1969), 25(2), 355-9

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal

LANGUAGE:

SOURCE:

English

AΒ Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

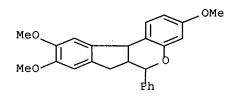
IT 21834-73-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

21834-73-1 CAPLUS RN

Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6-CNphenyl- (8CI) (CA INDEX NAME)



ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER:

40:23981

ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b

TITLE: Condensation of tetraphenylbutynediol with phenol

AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.

CORPORATE SOURCE: Leningrad Chem. Tech. Inst.

SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: English

[.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 q. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yelloworange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7°, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et20 was treated with 22.5 g. PCl3 at 1° over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT 860186-11-4P, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11triphenyl-

RL: PREP (Preparation)

(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)

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ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:381028 CAPLUS Full-text

DOCUMENT NUMBER:

144:432681

TITLE:

Preparation of substituted benzopyrans as selective

estrogen receptor-beta agonists

INVENTOR(S):

Norman, Bryan Hurst; Richardson, Timothy Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 50 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

1	PATENT NO.							KIND DATE											
	WO	0 2006044176						2006	0427				20051005						
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		w:																	
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PRIOR	PRIORITY APPLN. INFO.:									1	US 2	004-	6196	27P	P 20041018				
	<b>*</b> •									1	WO 2	005-1	US35	472	1	W 2	0051	005	
OTHER	OTHER SOURCE(S):																		

ΙI

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GI

Title compds. represented by the formula I [wherein R = halo, alkyl or R3- (CH2)m; G = 0, CF2, SOn, CO, CR1H or CR2(OH); R1 = F, OH, cyano, etc.; R2 = CF3 or alkyl; R3 = CN, OH, alkenyl or alkoxy(carbonyl); m = 0-2; n = 0-2; and pharmaceutical acceptable salts thereof] were prepared as estrogen receptor-beta (ER- $\beta$ ) agonists. For example, II was given in a multi-step synthesis starting from 3-bromo-2-hydroxy-5- methoxybenzaldehyde. I exhibited binding affinities (Kis) at the ER- $\alpha$  subtype in the range 4- >1000 nM and to the ER- $\beta$  subtype in the range of 0.3-120 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of ER- $\beta$  mediated diseases, such as prostate cancer or benign prostate hyperplasia (no data).

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted benzopyrans as selective estrogen receptor-beta agonists)

RN 885025-43-4 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 6-ethenyl-2,2-difluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2005:369613 CAPLUS Full-text

DOCUMENT NUMBER:

144:150207

TITLE:

Traceless solid-phase synthesis of

cyclopenta[c]quinolines and cyclopenta[c]chromenes via

hetero [6+3] cycloadditions of fulvene. A facile

approach to the 11-heterosteroids framework

AUTHOR(S):

Hong, Bor-Cherng; Chen, Zhong-Yi; Chen, Wei-Hung; Sun,

Hsu-I.; Lee, Gene-Hsiang

CORPORATE SOURCE:

Department of Chemistry and Biochemistry, National

Chung Cheng University, Chia-Yi, 621, Taiwan

SOURCE:

Journal of the Chinese Chemical Society (Taipei,

Taiwan) (2005), 52(1), 181-200

PUBLISHER:

CODEN: JCCTAC; ISSN: 0009-4536

POGINGIA GUDG

Chinese Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 144:150207

GI

$$R^2$$
 $R^3$ 
 $R^3$ 

The hetero [6+3] cycloaddn. of resin-bound fulvenes I (X = resin; R1 = H, Me; R2 = H, Me, Et, n-Pr, n-Bu, Ph) to benzoquinones and quinonimines, e.g. II (Y = O, 4-Me2NC6H4N; R3 = H, Me, Cl), provides an efficient route to the synthesis of cyclopenta[c]chromenes and cyclopenta[c]quinolines, e.g. III. The structure of the cyclopenta[c]chromene skeleton was confirmed by the X-ray structure anal. of the 4-bromobenzoate of III (Y = O; R1 = H; R2 = R3 = Me). The antiproliferative activity of two cyclopenta[c]chromene derivs. against a number of carcinogenic human cell lines has been studied.

IT 874118-35-1P 874118-44-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(solution-phase and traceless solid-phase synthesis of hydroxy-substituted cyclopenta[c]quinolines and cyclopenta[c]chromenes via hetero [6+3] cycloaddns. of fulvenes with quinones or quinonimines)

RN 874118-35-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI) (CA INDEX NAME)

RN 874118-44-2 CAPLUS
CN Cyclopenta[d]naphtho[1,2-b]pyran-11-ol, 6-phenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:927190 CAPLUS Full-text

DOCUMENT NUMBER:

141:395410

TITLE:

Preparation of substituted benzopyrans as selective

estrogen receptor-beta agonists

INVENTOR(S):

Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer,

Lance Allen; Richardson, Timothy Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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WO	2004	2004094400			A3 20050224														
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		TD,											·	•	·	•	·		
AU	2004	2327	98		A1	2004	1104	AU 2004-232798						20040408					
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											, HU,				•	•	•		
BR	2004	0095	88		Α		2006	0418	•	BR 2	2004-	9588			2	0040	408		
CN	1777	614			Α						2004-								
JP	2006	5242									2006-								
US	US 2007106082										2005-					0051	006		
MX	2005	PA11	243		Α		2005	1215		MX 2	2005-	PA11:	243		2	0051	019		
PRIORITY											2003-					0030			
											2004-1					0040			
OTHER SO	OTHER SOURCE(S):						141:	3954					-		_				

GI

Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multistep synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER- $\alpha$  subtype in the range 5.0 - >10,000 nM and to the ER- $\beta$  subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT 787621-81-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-88-9 CAPLUS

CN

Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787621-99-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 787622-40-6 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RN 787622-43-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-78-0 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

### IT 787622-29-1P 787622-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787622-29-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-41-7 CAPLUS

CN Silane, (1,1-dimethylethyl) [4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2-[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

Me Ne

ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2003:417738 CAPLUS Full-text

DOCUMENT NUMBER:

139:6768

TITLE:

Preparation of benzopyran derivatives as selective

estrogen receptor  $\beta$  agonists

INVENTOR(S):

Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar,

Charles Willis, III; Neubauer, Blake Lee; Norman,

Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy

Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 138 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

FAMILY ACC. NUM. COUNT:

English

PATENT INFORMATION:

PA	PATENT NO.						KIND DATE			PLI	CAT:	ION 1	DATE						
WC	2003	2003044006					2003	0530	WO	20	002-T	JS33	20021107						
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CA	4 2467				A1				CA						2	0021	107		
Αl	J 2002	3592	83		A1				AU					20021107					
E	1448	544			A1								20021107 .						
. EI	1448	1448544					2007												
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CN	1 1589								CN				20021107						
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JI	2005	5130	27		T		2005	0512	JP	20	003-	5456	20021107						
NZ	3 5318	50			Α		2007	0126	NZ	20	002-5	5318	20021107						
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									TR, A								•		
ΓA	3624				T		2007					7938			2	0021	107		
US	2004	2491	67		<b>A1</b>		2004	1209	US	20	04-4	1930	20040420						
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IN	2004	KN00	639		Α		2006	0421	IN	04-1	CN63	9		2	0040	517			
. <b>M</b> X	2004	PA04	703				2004	0819	MX	20	04-1	PA47	03		2	0040	518		
NC	2004	0025	83		A A		2004	0618	NO	04-2	2583		20040618						
PRIORIT	Y APP	LN.	INFO					•	US	01-3	3327	P 20011119							
													22P			0020			
													06			0021	107		

MARPAT 139:6768

The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor  $\beta$  agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor  $\beta$  (ER  $\beta$ ) with a Ki of <1 nM and Ki(ER  $\alpha$ )/Ki(ER  $\beta$ ) of 8.0. IT 533884-11-6P

III

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor  $\beta$  agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benz opyran-4-yl]- (9CI) (CA INDEX NAME)

ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN L6

ACCESSION NUMBER: 1998:689997 CAPLUS Full-text

DOCUMENT NUMBER: 130:38272

A novel tandem bicyclization to form an indenopyran TITLE:

ring system

AUTHOR (S): Chakraborty, Manisha; McConville, David B.; Saito,

Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier,

Claire A.; Youngs, Wiley J.

Dep. of Chemistry, University of Akron, Akron, OH, CORPORATE SOURCE:

44325-3601, USA

SOURCE: Tetrahedron Letters (1998), 39(45), 8237-8340

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:38272

A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization AB between alkyne and hydroxy functionality of an alkynyl hydroquinone has been

observed to give a highly conjugated ring system.

IT 216777-12-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of indenopyrans by tandem bicyclization)

RN 216777-12-7 CAPLUS

CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) NAME).

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN 1972:152831 CAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER: 76:152831

TITLE: Condensation of phenyl ethynyl ketone with

cyclopentadiene. Reinvestigation

AUTHOR (S): Venkataramani, P. S.; Chandrasekharan, S.;

Swaminathan, S.

CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India

SOURCE: Tetrahedron (1972), 28(5), 1249-55

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

For diagram(s), see printed CA Issue.

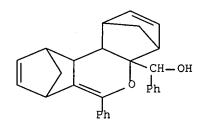
AB The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT 36144-49-7P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10bhexahydro- $\alpha$ , 6-diphenyl-,  $[1\alpha, 4\alpha, 4a\beta(R^*), 7\beta, 10$ . beta.,  $10a\alpha$ ,  $10b\beta$ ] - (9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 8. CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1969:77707 CAPLUS Full-text

DOCUMENT NUMBER:

70:77707

TITLE:

Experiments in the brazilane series. I. Preparation

of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR (S):

SOURCE:

Morsingh, Francis

CORPORATE SOURCE:

Univ. Malaya, Kuala Lumpur, Malay. Tetrahedron (1969), 25(2), 355-9

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal

LANGUAGE: English

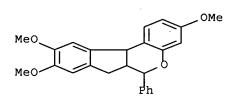
AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT 21834-73-1P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

ВИ 21834-73-1 CAPLUS

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6phenyl- (8CI) (CA INDEX NAME)



CAPLUS COPYRIGHT 2007 ACS on STN ANSWER 8 OF 8

ACCESSION NUMBER:

1946:23981 CAPLUS Full-text

DOCUMENT NUMBER:

40:23981

ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b

TITLE: Condensation of tetraphenylbutynediol with phenol AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.

CORPORATE SOURCE: Leningrad Chem. Tech. Inst.

SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: English

AB [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 q. 1diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yelloworange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7 °, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et20 was treated with 22.5 g. PCl3 at 1° over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194- $5^{\circ}$  (0.2 g.), and m.  $165^{\circ}$  (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfamilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT 860186-11-4P, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11triphenyl-

RL: PREP (Preparation)

(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)

=>

=> file reg

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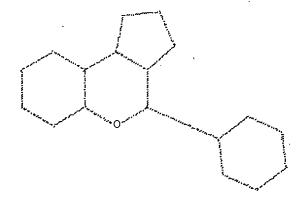
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L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17 sss sam

SAMPLE SEARCH INITIATED 15:13:58 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -1636 TO ITERATE

100.0% PROCESSED

1636 ITERATIONS

17 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE

\*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

30294 TO 35146

PROJECTED ANSWERS:

93 TO 587

=> d scan

L8

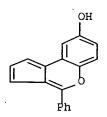
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IN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI)

17 SEA SSS SAM L7

MF C18 H12 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L8 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN IN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9bhexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI)
MF C19 H16 F2 O3

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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FULL SEARCH INITIATED 15:15:04 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 31330 TO ITERATE

100.0% PROCESSED 31330 ITERATIONS SEARCH TIME: 00.00.01

281 ANSWERS

L9 281 SEA SSS FUL L7

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COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by
structure-building or screen commands and text search terms. L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles. The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

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'2004' NOT A VALID FIELD CODE

'2004' NOT A VALID FIELD CODE

'2004' NOT A VALID FIELD CODE

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=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 175.25 290.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

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=> s 17 and (py<2004 or ay<2004 or pry<2004)
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Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

17 ANSWERS

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SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED 1636 ITERATIONS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 30294 TO 35146 PROJECTED ANSWERS: 93 TO 587

L11 17 SEA SSS SAM L7

L12 8 L11

SEARCH TIME: 00.00.01

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L13 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:927190 CAPLUS Full-text

DOCUMENT NUMBER:

141:395410

TITLE:

Preparation of substituted benzopyrans as selective

estrogen receptor-beta agonists

INVENTOR(S):

Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer,

Lance Allen; Richardson, Timothy Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA PCT Int. Appl., 129 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA						D -	DATE		APPLICATION NO.							DATE			
	2004094400				A2 20041104			WO 2004-US9272						20040408 <					
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							DE,												
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EF	1626	5974			A2		2006	0222	]	EP 2	004-	7597	67		2	0040	408	<	
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,		
							TR,							•	•	•	•		
BF	2004	10095	88		Α		2006	0418	1	BR 2	004-	20040408 <							
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JI	2006	55242	40		Т		2006	1026	1	JP 2	006-	5093:	32			00404			
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MX	2009	PA11	243		Α		2005				005-					0051			
PRIORIT	Y API	PLN.	INFO	. :							003-		-			00304			
																00404		•	
THER S	HER SOURCE(S):					WO 2004-US9272 W 20040408 MARPAT 141:395410													

GI

Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multistep synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER- $\alpha$  subtype in the range 5.0 - >10,000 nM and to the ER- $\beta$  subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT 787621-81-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
agonists)

RN 787621-88-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787621-99-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 787622-40-6 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RN 787622-43-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-78-0 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

### IT 787622-29-1P 787622-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787622-29-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-41-7 CAPLUS

Relative stereochemistry.

Me Ne

L13 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS ON STN ACCESSION NUMBER: 2003:417738 CAPLUS Full-text

DOCUMENT NUMBER:

139:6768

TITLE:

Preparation of benzopyran derivatives as selective

estrogen receptor  $\beta$  agonists

Eli Lilly and Company, USA

INVENTOR(S):

Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar, Charles Willis, III; Neubauer, Blake Lee; Norman,

Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy

Ivo

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 138 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	PATENT NO.									APPLICATION NO.						DATE			
WO.	2003	A1 20030530					 WO 21	 002-1	US33	 622		20021107 <							
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																	311 <		
										EP 2	002-	7938	06		A3 2	0021	107 <	-	

OTHER SOURCE(S):

MARPAT 139:6768

The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor  $\beta$  agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor  $\beta$  (ER  $\beta$ ) with a Ki of <1 nM and Ki(ER  $\alpha$ )/Ki(ER  $\beta$ ) of 8.0. IT 533884-11-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor  $\beta$  agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benz opyran-4-yl]- (9CI) (CA INDEX NAME)

L13 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:689997 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 130:38272

TITLE: A novel tandem bicyclization to form an indenopyran

ring system

AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito,

Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier,

Claire A.; Youngs, Wiley J.

CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH,

44325-3601, USA

SOURCE: Tetrahedron Letters (1998), 39(45),

8237-8340

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been

observed to give a highly conjugated ring system.

IT 216777-12-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of indenopyrans by tandem bicyclization)

RN 216777-12-7 CAPLUS

CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1972:152831 CAPLUS Full-text

DOCUMENT NUMBER: 76:152831

TITLE: Condensation of phenyl ethynyl ketone with

cyclopentadiene. Reinvestigation

AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.;

Swaminathan, S.

CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India

SOURCE: Tetrahedron (1972), 28(5), 1249-55

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

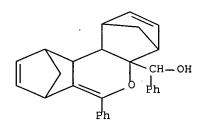
AB The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(0)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT 36144-49-7P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

36144-49-7 CAPLUS RN

1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-CN hexahydro- $\alpha$ , 6-diphenyl-, [1 $\alpha$ , 4 $\alpha$ , 4 $\alpha$ β (R\*), 7 $\beta$ , 10. beta.,  $10a\alpha$ ,  $10b\beta$ ] - (9CI) (CA INDEX NAME)



CAPLUS COPYRIGHT 2007 ACS on STN L13 ANSWER 5 OF 6

ACCESSION NUMBER:

1969:77707 CAPLUS Full-text

DOCUMENT NUMBER:

70:77707

TITLE:

SOURCE:

Experiments in the brazilane series. I. Preparation

of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S):

Morsingh, Francis

CORPORATE SOURCE:

Univ. Malaya, Kuala Lumpur, Malay. Tetrahedron (1969), 25(2), 355-9

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

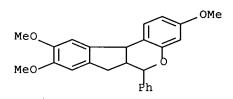
IT 21834-73-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN21834-73-1 CAPLUS

CNBenz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6phenyl- (8CI) (CA INDEX NAME)



L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER:

40:23981

ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b

TITLE: Condensation of tetraphenylbutynediol with phenol AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.

CORPORATE SOURCE: Leningrad Chem. Tech. Inst.

SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: English

· AB [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yelloworange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7°, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et20 was treated with 22.5 g. PCl3 at 1° over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194- $5^{\circ}$  (0.2 g.), and m.  $165^{\circ}$  (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfamilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT 860186-11-4P, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11triphenyl-

RL: PREP (Preparation)

(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)

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NEWS 10 JUN 29
                 STN Viewer now available
NEWS 11
         JUN 29
                 STN Express, Version 8.2, now available
NEWS 12 JUL 02
                 LEMBASE coverage updated
NEWS 13 JUL 02 LMEDLINE coverage updated
NEWS 14 JUL 02 SCISEARCH enhanced with complete author names
NEWS 15 JUL 02
                 CHEMCATS accession numbers revised
NEWS 16 JUL 02
                 CA/CAplus enhanced with utility model patents from China
NEWS 17 JUL 16 CAplus enhanced with French and German abstracts
NEWS 18 JUL 18 CA/CAplus patent coverage enhanced
NEWS 19 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20 JUL 30 USGENE now available on STN
NEWS 21 AUG 06 CAS REGISTRY enhanced with new experimental property tags
                 BEILSTEIN updated with new compounds
NEWS 22 AUG 06
NEWS 23 AUG 06 FSTA enhanced with new thesaurus edition
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NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

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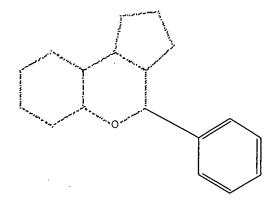
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100.0% PROCESSED

1636 ITERATIONS

17 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

30294 TO 35146

PROJECTED ANSWERS:

93 TO 587

L2

17 SEA SSS SAM L1

=> d scan

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI)

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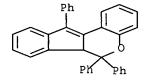
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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI)

MF C34 H24 O



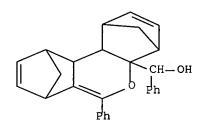
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#### HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10b-hexahydro- $\alpha$ ,6-diphenyl-, [1 $\alpha$ ,4 $\alpha$ ,4a $\beta$ (R\*),7 $\beta$ ,10. beta.,10a $\alpha$ ,10b $\beta$ ]- (9CI)

MF C28 H26 O2



### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

## HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI)

MF C32 H30 O4

Relative stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI)

MF C18 H12 O2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-

tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI)

MF C32 H26 O4

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

## HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9bhexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI)

MF C19 H16 F2 O3

Absolute stereochemistry.

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

### HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Cyclopenta[d]naphtho[1,2-b]pyran-11-ol, 6-phenyl- (9CI)

MF C22 H14 O2

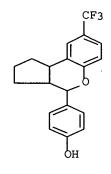
#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

# HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

IN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benz
opyran-4-yl]- (9CI)

MF C19 H17 F3 O2



# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

# HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN

MF C35 H54 O3 Si3

Relative stereochemistry.

PAGE 2-A

ме ме

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=>

Uploading C:\Program Files\Stnexp\Queries\10-552504a.str

# L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 13 sss sam

SAMPLE SEARCH INITIATED 14:43:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2835 TO ITERATE

70.5% PROCESSED 2000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

53507 TO 59893

PROJECTED ANSWERS:

0 TO (

L4 0 SEA SSS SAM L3

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

13.95 14.16

FILE 'CAPLUS' ENTERED AT 14:45:00 ON 06 AUG 2007
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FILE COVERS 1907 - 6 Aug 2007 VOL 147 ISS 7 FILE LAST UPDATED: 5 Aug 2007 (20070805/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 12 and (py<2004 or ay<2004 or pry<2004)

8 L2

23927525 PY<2004

4731037 AY<2004

4212934 PRY<2004

L5 6 L2 AND (PY<2004 OR AY<2004 OR PRY<2004)

=> d scan

L5 6 ANSWERS CAPLUS COPYRIGHT 2007 ACS on STN

IC ICM C07D311-00

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CC
    27-7 (Heterocyclic Compounds (One Hetero Atom))
    Section cross-reference(s): 1, 63
ΤI
    Preparation of substituted benzopyrans as selective estrogen receptor-beta
    agonists
ST
    benzopyran prepn estrogen receptor beta agonist anticancer
IT
    Prostate gland, disease
        (benign hyperplasia; preparation of cyclopenta[c]chromenols as selective
       estrogen receptor-beta agonists)
ΙT
    Hyperplasia
        (benign prostatic; preparation of cyclopenta[c]chromenols as selective
       estrogen receptor-beta agonists)
IT
    Prostate gland, neoplasm
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
       agonists)
IT
    Antitumor agents
        (prostate gland; preparation of cyclopenta[c]chromenols as selective
        estrogen receptor-beta agonists)
ΙT
    Estrogen receptors
    RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (β; preparation of cyclopenta[c]chromenols as selective estrogen
       receptor-beta agonists)
                                   787621-80-1P 787621-81-2P
IT
    787621-59-4P
                    787621-60-7P
    787622-06-4P
                    787622-10-0P
                                   787622-73-5P
    RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
    preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
        agonists)
IT
    787621-53-8P
                   787621-54-9P
                                   787621-55-0P
                                                 787621-56-1P
                                                                787621-57-2P
    787621-58-3P
                   787621-61-8P
                                  787621-62-9P
                                                 787621-63-0P
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    787621-69-6P
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                   787622-44-0P
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    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
    (Uses)
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
       agonists)
    62-23-7, p-Nitrobenzoic acid
                                  75-86-5, Acetone cyanohydrin
    Methyl acrylate
                     96-35-5, Methyl glycolate
                                                  100-39-0, Benzyl bromide
                                         623-82-5, (R)-(+)-3-Methyladipic acid
    123-31-9, Hydroquinone, reactions
    892-20-6, Triphenyltin hydride
                                    1066-54-2, Trimethylsilylacetylene
    1100-88-5, Benzyltriphenylphosphonium chloride
                                                     1530-32-1,
    Ethyltriphenylphosphonium bromide
                                       2365-48-2, Methyl thioglycolate
    2622-05-1, Allylmagnesium chloride 3058-01-3, 3-Methyladipic acid
    5781-53-3, Methyl chloroglyoxylate 6228-47-3, Propyltriphenylphosphonium
              6793-92-6, p-Benzyloxybromobenzene
                                                   10347-88-3,
    3-tert-Butyladipic acid 10538-51-9, 2,5-Dimethoxycinnamic acid
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22444-89-9, Butyltriphenylphosphonium 25458-45-1, 1-Bromo-4-
     (methoxymethoxy) benzene 37595-74-7, N-Phenyltrifluoromethanesulfonimide
     38053-91-7, 2-[(Trimethylsilyl)oxy]butadiene
                                                   38078-09-0,
     N,N-Diethylaminosulfur trifluoride 70160-51-9
                                                      72047-94-0,
     [2-(Acetoxymethyl)allyl]trimethylsilane
                                              108270-19-5
     4-(Benzyloxy)phenylboronic acid 787622-05-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
        agonists)
IT
     2689-68-1P
                 4463-74-5P
                              6093-68-1P, 6-Hydroxycoumarin
                                                              57595-23-0P
     87905-74-6P, 1,4-Bis (methoxymethoxy) benzene
                                                  608536-53-4P,
     6-Methoxymethoxycoumarin
                              787621-46-9P
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                                  787622-20-2P
                                                 787622-21-3P 787622-23-5P.
     6-Benzyloxychromen-2-one 787622-25-7P 787622-26-8P 787622-27-9P
     787622-28-0P 787622-29-1P
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                                                                787622-67-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    (Reactant or reagent)
        (preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta
        agonists)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
L5
      6 ANSWERS
                 CAPLUS COPYRIGHT 2007 ACS on STN
CC
     10 (Organic Chemistry)
ΤI
     Condensation of tetraphenylbutynediol with phenol
IT
     Catalysts
        (for condensation, of PhOH with 1,1,4,4-tetraphenyl-2-butyne-1,4-diol)
IT
     411220-98-9P, Indene, 1-benzohydrylidene-2-chloro-3-phenyl-
     411220-98-9P, Methane, (2-chloro-3-phenyl-1-indenylidene)diphenyl-
     854748-48-4P, Methane, [2-(p-methoxyphenyl)-3-phenyl-1-
     indenylidene]diphenyl- 854748-48-4P, Anisole, p-(1-benzohydrylidene-3-
     phenyl-2-indenyl) - 854748-48-4P, Indene, 1-benzohydrylidene-2-(p-
     methoxyphenyl)-3-phenyl- 854749-76-1P, Indene, 1-benzohydrylidene-2-
     phenoxy-3-phenyl-
                        854749-76-1P, Methane, (2-phenoxy-3-phenyl-1-
     indenylidene)diphenyl- 860000-10-8P, Furan, 2,5-dihydro-3-phenoxy-
     2,2,5,5-tetraphenyl- 860186-11-4P, Benz[b]indeno[2,1-d]pyran,
     6,6a-dihydro-6,6,11-triphenyl- 861008-63-1P, Phenol,
     p-(1-benzohydrylidene-3-phenyl-2-indenyl)-
    RL: PREP (Preparation)
        (preparation of)
IT
     1483-74-5, 2-Butyne-1,4-diol, tetraphenyl-
        (reaction with phenol)
IT
     108-95-2, Phenol
        (reactions of, with 1,1,4,4-tetraphenyl-2-butyne-1,4-diol)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0
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YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y
L5
    ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN
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ACCESSION NUMBER:

2004:927190 CAPLUS Full-text

DOCUMENT NUMBER:

141:395410

TITLE:

Preparation of substituted benzopyrans as selective

estrogen receptor-beta agonists

INVENTOR(S):

Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer,

Lance Allen; Richardson, Timothy Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 129 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

I ANCHACE.

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.						KIND DATE								,				
	2004094400							WO 2004-US9272										
WO	2004094400			A3 20050224			0224											
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KZ,	LC,	
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THER S	OURCE	(S):			MAR	PAT	141:	3954		2	004	0072	, 2		. 21	. 040-	± 0 0	

GI

Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multistep synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER- $\alpha$  subtype in the range 5.0 - >10,000 nM and to the ER- $\beta$  subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT 787621-81-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-88-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787621-99-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 787622-40-6 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RN 787622-43-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-78-0 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

### IT 787622-29-1P 787622-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists).

RN 787622-29-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-41-7 CAPLUS

CN Silane, (1,1-dimethylethyl) [4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

46 No

L5 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2003:417738 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER:

139:6768

TITLE:

Preparation of benzopyran derivatives as selective

estrogen receptor  $\beta$  agonists

INVENTOR(S):

Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar,

Charles Willis, III; Neubauer, Blake Lee; Norman,

Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy

Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 138 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

WO 2003044006 A1 20030530 WO 2002-US33622 200 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,	GE, GH,				
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, G	GE, GH,				
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GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,	T.K. T.R.				
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ,	OM, PH,				
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR,					
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, A	AZ, BY,				
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	040518 <				
NO 2004002583 A 20040618 NO 2004-2583 206	040618 <				
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US 2002-363622P P 200	020311 <				
EP 2002-793806 A3 200	021107 <				

MARPAT 139:6768

AB The title compds: I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor  $\boldsymbol{\beta}$ agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor  $\beta$  (ER  $\beta$ ) with a Ki of <1 nM and Ki(ER  $\alpha$ )/Ki(ER  $\beta$ ) of 8.0. TT 533884-11-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor  $\beta$  agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benz opyran-4-yl] - (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:689997 CAPLUS Full-text

DOCUMENT NUMBER: 130:38272

TITLE: A novel tandem bicyclization to form an indenopyran

ring system

AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito,

Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier,

Claire A.; Youngs, Wiley J.

CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH,

44325-3601, USA

SOURCE: Tetrahedron Letters (1998), 39(45),

8237-8340

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been

observed to give a highly conjugated ring system.

IT 216777-12-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of indenopyrans by tandem bicyclization)

RN 216777-12-7 CAPLUS

CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1972:152831 CAPLUS Full-text

DOCUMENT NUMBER: 76:152831

LANGUAGE:

TITLE: Condensation of phenyl ethynyl ketone with

cyclopentadiene. Reinvestigation

AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.;

Swaminathan, S.

CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India

SOURCE: Tetrahedron (1972), 28(5), 1249-55

English

CODEN: TETRAB: ISSN: 0040-4020

DOCUMENT TYPE: Journal

GI For diagram(s), see printed CA Issue.

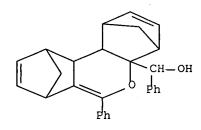
The earlier structural assignment of 2-benzoylnorborna-diene (I) for the AB product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

TT36144-49-7P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10bhexahydro- $\alpha$ , 6-diphenyl-,  $[1\alpha, 4\alpha, 4a\beta(R^*), 7\beta, 10]$ . beta.,  $10a\alpha$ ,  $10b\beta$ ] - (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1969:77707 CAPLUS Full-text

DOCUMENT NUMBER: 70:77707

TITLE: Experiments in the brazilane series. I.

of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S): Morsingh, Francis

CORPORATE SOURCE: Univ. Malaya, Kuala Lumpur, Malay. SOURCE:

Tetrahedron (1969), 25(2), 355-9

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The

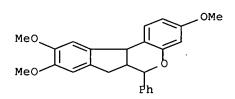
synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT 21834-73-1P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 21834-73-1 CAPLUS

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6phenyl- (8CI) (CA INDEX NAME)



ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER: 40:23981 ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b

TITLE: Condensation of tetraphenylbutynediol with phenol

AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.

CORPORATE SOURCE: Leningrad Chem. Tech. Inst.

SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: English

AΒ [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yelloworange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7°, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et20 was treated with 22.5 q. PC13 at 1°over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT 860186-11-4P, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11triphenyl-

RL: PREP (Preparation)

(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)

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L6 8 L2
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YOU HAVE REQUESTED DATA FROM 8 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2006:381028 CAPLUS Full-text

DOCUMENT NUMBER:

144:432681

TITLE:

Preparation of substituted benzopyrans as selective

estrogen receptor-beta agonists

INVENTOR(S):

Norman, Bryan Hurst; Richardson, Timothy Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

GI

PCT Int. Appl., 50 pp.

CODEN: PIXXD2 Patent

DOCUMENT TYPE: LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.						KIND DATE					ICAT:		DATE					
WO	WO 2006044176				A1	_	2006	20060427					20	0051	005			
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KP,	KR,	ΚZ,	
		LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	
		NA,	NG,	NI,	NO,	ΝZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	
		SK,	SL,	SM,	SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	
		YU,	ZA,	ZM,	ZW													
	RW:	AT,	ΒE,	ВG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	
		IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,	
		GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,	
		KG,	ΚZ,	MD,	RU,	TJ,	TM											
CA	2578	300			A1		2006	0427	(	CA 2	005-2	2578		20051005				
EP	1805	160			<b>A</b> 1		2007	0711	]	EP 2	005-	8074	48		20	0051	005	
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		IS,	IT,	LI,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR		
PRIORITY	Y APP	LN.	INFO	. :					1	US 2	004-0	6196:	27P	]	P 20	0041	018	
									1	WO 2	005-1	JS354	472	1	W 20	0051	005	
OTHER SO	MARPAT 144:432681																	

Ι

ΙI

AΒ Title compds. represented by the formula I [wherein R = halo, alkyl or R3-(CH2)m; G = O, CF2, SOn, CO, CR1H or CR2(OH); R1 = F, OH, Cyano, etc.; R2 =CF3 or alkyl; R3 = CN, OH, alkenyl or alkoxy(carbonyl); m = 0-2; n = 0-2; and pharmaceutical acceptable salts thereof] were prepared as estrogen receptorbeta  $(ER-\beta)$  agonists. For example, II was given in a multi-step synthesis starting from 3-bromo-2-hydroxy-5- methoxybenzaldehyde. I exhibited binding affinities (Kis) at the ER- $\alpha$  subtype in the range 4- >1000 nM and to the ER- $\beta$ subtype in the range of 0.3-120 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of ER-β mediated diseases, such as prostate cancer or benign prostate hyperplasia (no data). TТ 885025-43-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of substituted benzopyrans as selective estrogen receptor-beta agonists)

RN 885025-43-4 CAPLUS

> Cyclopenta[c][1]benzopyran-8-ol, 6-ethenyl-2,2-difluoro-1,2,3,3a,4,9bhexahydro-4-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN L<sub>6</sub>

ACCESSION NUMBER:

2005:369613 CAPLUS Full-text

DOCUMENT NUMBER:

144:150207

TITLE:

CN

Traceless solid-phase synthesis of

cyclopenta[c]quinolines and cyclopenta[c]chromenes via

hetero [6+3] cycloadditions of fulvene. A facile

approach to the 11-heterosteroids framework

AUTHOR (S):

Hong, Bor-Cherng; Chen, Zhong-Yi; Chen, Wei-Hung; Sun,

Hsu-I.; Lee, Gene-Hsiang

CORPORATE SOURCE:

Department of Chemistry and Biochemistry, National

Chung Cheng University, Chia-Yi, 621, Taiwan

SOURCE:

Journal of the Chinese Chemical Society (Taipei,

Taiwan) (2005), 52(1), 181-200 CODEN: JCCTAC; ISSN: 0009-4536

PUBLISHER:

Chinese Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 144:150207

GI

$$R^{2}$$
 $R^{2}$ 
 $R^{3}$ 
 $R^{3}$ 
 $R^{3}$ 
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The hetero [6+3] cycloaddn. of resin-bound fulvenes I (X = resin; R1 = H, Me; R2 = H, Me, Et, n-Pr, n-Bu, Ph) to benzoquinones and quinonimines, e.g. II (Y = O, 4-Me2NC6H4N; R3 = H, Me, Cl), provides an efficient route to the synthesis of cyclopenta[c]chromenes and cyclopenta[c]quinolines, e.g. III. The structure of the cyclopenta[c]chromene skeleton was confirmed by the X-ray structure anal. of the 4-bromobenzoate of III (Y = O; R1 = H; R2 = R3 = Me). The antiproliferative activity of two cyclopenta[c]chromene derivs. against a number of carcinogenic human cell lines has been studied.

IT 874118-35-1P 874118-44-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (solution-phase and traceless solid-phase synthesis of hydroxy-substituted cyclopenta[c]quinolines and cyclopenta[c]chromenes via hetero [6+3] cycloaddns. of fulvenes with quinones or quinonimines)

RN 874118-35-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI) (CA INDEX NAME)

RN 874118-44-2 CAPLUS

CN Cyclopenta[d]naphtho[1,2-b]pyran-11-ol, 6-phenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER:

2004:927190 CAPLUS Full-text

DOCUMENT NUMBER:

141:395410

TITLE:

Preparation of substituted benzopyrans as selective

estrogen receptor-beta agonists

INVENTOR(S):

Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer,

Lance Allen; Richardson, Timothy Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

GI

PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA'	TENT :	NO.			KIN	D	DATE			APPI	ICAT	ION :	NO.		Ι	ATE	
WO	2004	0944	00		A2	-	2004	1104		WO 2	2004 -	US92	 72		2	0040	408
WO	2004	0944	00		<b>A</b> 3		2005	0224									
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											EC,						
											JP,						
				-	-	-			•		MK,	•	•	•	•	•	•
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	RW:										SZ,						
											BG,						
									-	-	MC,		-		•	•	•
						-	-	•			GN,		•	•		•	•
		TD,				,	,	,	,	,		- 21		,	,	,	,
AU	2004	2327:	98		A1		2004	1104		AU 2	004 -	2327	98		2	0040	408
CA	2518	819			A1 20041104			CA 2004-2518819						0040			
ĒP						0222	EP 2004-759767					20040408					
	R:	AT,	BE,	CH.	DE.						IT,						
											HU,			,	~-,	,	,
BR	2004		•		•	•	•	•	•		004-	,			2	0040	408
									CN 2004-80010817								
JР	JP 2006524240									JP 2006-509332				20040408			
US	2007	1060	82		A1						005-					0051	
MX	MX 2005PA11243																
	PRIORITY APPLN. INFO.:										003-					0030	
											004-1	-				0040	
OTHER SO		MAR	PAT	141:	3954	10											

Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multistep synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER- $\alpha$  subtype in the range 5.0 - >10,000 nM and to the ER- $\alpha$  subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT 787621-81-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

ΙI

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-88-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787621-99-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 787622-40-6 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RN 787622-43-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-78-0 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CAINDEX NAME)

## IT 787622-29-1P 787622-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787622-29-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-41-7 CAPLUS

Relative stereochemistry.

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L6 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2003:417738 CAPLUS Full-text

DOCUMENT NUMBER:

139:6768

TITLE:

Preparation of benzopyran derivatives as selective

estrogen receptor  $\boldsymbol{\beta}$  agonists

INVENTOR(S):

Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar,

Charles Willis, III; Neubauer, Blake Lee; Norman,

Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy

Ivc

PATENT ASSIGNEE(S):

SOURCE:

Eli Lilly and Company, USA

PCT Int. Appl., 138 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				APPLICATION NO.					
WO 2003044	006	A1		WO 2002-US33622					
W: AE	AG, AL,	AM, AT	r, AU, AZ,	BA, BB, BG, BR, BY,	BZ, CA, CH, CN,				
				DZ, EC, EE, ES, FI,					
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LS	LT, LU,	LV, MA	A, MD, MG,	MK, MN, MW, MX, MZ,	NO, NZ, OM, PH,				
PL.	PT, RO,	RU, SI	O, SE, SG,	SI, SK, SL, TJ, TM,	TN, TR, TT, TZ,				
UA	UG, US,	UZ, VC	C, VN, YU,	ZA, ZM, ZW					
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KG	KZ, MD,	RU, TJ	J, TM, AT,	BE, BG, CH, CY, CZ,	DE, DK, EE, ES,				
FI	FR, GB,	GR, IE	E, IT, LU,	MC, NL, PT, SE, SK,	TR, BF, BJ, CF,				
CG	CI, CM,	GA, GN	1, GQ, GW,	ML, MR, NE, SN, TD,	TG				
CA 2467013		A1	20030530	CA 2002-2467013	20021107				
AU 2002359:	283	A1	20030610	AU 2002-359283	20021107				
EP 1448544		A1	20040825	EP 2002-793806	20021107				
EP 1448544									
R: AT	BE, CH,	DE, DE	K, ES, FR,	GB, GR, IT, LI, LU,	NL, SE, MC, PT,				
IE	SI, LT,	LV, FI	I, RO, MK,	CY, AL, TR, BG, CZ,	EE, SK				
CN 1589268		Α	20050302	CN 2002-822991	20021107				
HU 2004026	28	A2		HU 2004-2628	20021107				
JP 2005513	27	T		JP 2003-545643	20021107				
NZ 531850		A		NZ 2002-531850	20021107				
EP 1790644		A1		EP 2007-102693	20021107				
				DK, EE, ES, FI, FR,					
LI	LU, MC,	NL, PI	r, se, sk,	TR, AL, LT, LV, MK,	RO, SI				
AT 362471		T	20070615	AT 2002-793806	20021107				
US 2004249	L67	A1	20041209	US 2004-493092	20040420				
US 7217734		B2	20070515						
ZA 2004003	733	Α	20051004	ZA 2004-3733					
IN 2004KN0		Α	20060421	IN 2004-KN639	20040517				
MX 2004PA04	1703	Α	20040819	MX 2004-PA4703	20040518				
NO 2004002			20040618	NO 2004-2583	20040618				
PRIORITY APPLN.	INFO.:			US 2001-332766P					
			•	US 2002-363622P					
•				EP 2002-793806	A3 20021107				

MARPAT 139:6768

GI

The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor  $\beta$  agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor  $\beta$  (ER  $\beta$ ) with a Ki of <1 nM and Ki(ER  $\alpha$ )/Ki(ER  $\beta$ ) of 8.0. IT 533884-11-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor  $\boldsymbol{\beta}$  agonists)

RN 533884-11-6 CAPLUS

CN Phenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benz opyran-4-yl]- (9CI) (CA INDEX NAME)

L6 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:689997 CAPLUS Full-text

DOCUMENT NUMBER: 130:38272

TITLE: A novel tandem bicyclization to form an indenopyran

ring system

AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito,

Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier,

Claire A.; Youngs, Wiley J.

CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH,

44325-3601, USA

SOURCE: Tetrahedron Letters (1998), 39(45), 8237-8340

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:38272

AB A new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been

observed to give a highly conjugated ring system.

IT 216777-12-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of indenopyrans by tandem bicyclization)

RN 216777-12-7 CAPLUS

CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-

tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX

NAME)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1972:152831 CAPLUS Full-text

DOCUMENT NUMBER: 76:152831

TITLE: Condensation of phenyl ethynyl ketone with

cyclopentadiene. Reinvestigation

AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.;

Swaminathan, S.

CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India

SOURCE: Tetrahedron (1972), 28(5), 1249-55

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

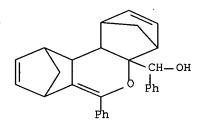
AΒ The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(0)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT 36144-49-7P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10bhexahydro- $\alpha$ , 6-diphenyl-,  $[1\alpha, 4\alpha, 4a\beta(R^*), 7\beta, 10$ . beta.,  $10a\alpha$ ,  $10b\beta$ ] - (9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN 1969:77707 CAPLUS Full-text

ACCESSION NUMBER:

DOCUMENT NUMBER: 70:77707

TITLE: Experiments in the brazilane series. I. Preparation

of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR(S): Morsingh, Francis

CORPORATE SOURCE: Univ. Malaya, Kuala Lumpur, Malay. SOURCE: Tetrahedron (1969), 25(2), 355-9

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

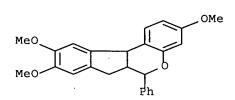
AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT 21834-73-1P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

21834-73-1 CAPLUS RN

CN Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6phenyl- (8CI) (CA INDEX NAME)



ANSWER 8 OF 8 L6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER: 40:23981 ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b

TITLE: Condensation of tetraphenylbutynediol with phenol

AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.

CORPORATE SOURCE: Leningrad Chem. Tech. Inst.

SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: English

[.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 g. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yelloworange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7°, by boiling with MeI in the presence of K2CO3 in Me2CO, or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et20 was treated with 22.5 g. PCl3 at 1° over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194- $5^{\circ}$  (0.2 g.), and m.  $165^{\circ}$  (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfamilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial AcOH. The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT 860186-11-4P, Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11triphenyl-

RL: PREP (Preparation)

(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)

=>

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL

FULL ESTIMATED COST ENTRY SESSION 101.43 115.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

CA SUBSCRIBER PRICE ENTRY SESSION -10.92 -10.92

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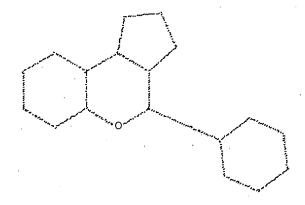
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L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

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100.0% PROCESSED

1636 ITERATIONS

17 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

30294 TO 35146

PROJECTED ANSWERS:

93 TO 587

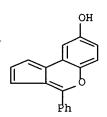
L8

17 SEA SSS SAM L7

=> d scan

L8 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN INCyclopenta[c][1]benzopyran-8-ol, 4-phenyl- (9CI)

MF C18 H12 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L8. 17 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN IN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9bhexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI)
MF C19 H16 F2 O3

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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FULL SCREEN SEARCH COMPLETED - 31330 TO ITERATE

100.0% PROCESSED 31330 ITERATIONS

SEARCH TIME: 00.00.01

L9 281 SEA SSS FUL L7

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COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by
structure-building or screen commands and text search terms. L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles. The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> s 19 and (py<2004 or ay<2004 or pry<2004)

'2004' NOT A VALID FIELD CODE

'2004' NOT A VALID FIELD CODE

'2004' NOT A VALID FIELD CODE

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0 PRY<2004

L10 0 L9 AND (PY<2004 OR AY<2004 OR PRY<2004)

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

281 ANSWERS

FULL ESTIMATED COST 175.25 290.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

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=> s 17 and (py<2004 or ay<2004 or pry<2004)
 REG1stry INITIATED</pre>

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SAMPLE SCREEN SEARCH COMPLETED - 1636 TO ITERATE

100.0% PROCESSED 1636 ITERATIONS

RATIONS 17 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 30294 TO 35146
PROJECTED ANSWERS: 93 TO 587

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L13 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

2004:927190 CAPLUS Full-text

DOCUMENT NUMBER:

141:395410

TITLE:

Preparation of substituted benzopyrans as selective

estrogen receptor-beta agonists

INVENTOR(S):

Durst, Gregory Lee; Norman, Bryan Hurst; Pfeifer,

Lance Allen; Richardson, Timothy Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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GI

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$$\longrightarrow$$
 OH I

Title compds. represented by the formula I [wherein G = CH-alkyl, CO, CHOH, CHCF3, CF2, C(OH)CF3, CH(OH)alkyl, CH-O-alkyl, CHOCO-alkyl, etc; and their enantiomers, and pharmaceutically acceptable salts thereof] were prepared as estrogen receptor (ER)-beta agonists. For example, II was given in a multistep synthesis starting from hydroquinone. I exhibited binding affinities (Kis) at the ER- $\alpha$  subtype in the range 5.0 - >10,000 nM and to the ER- $\beta$  subtype in the range of 0.20 - 429 nM. Thus, I and their pharmaceutical compns. are useful as estrogen receptor agonists for the treatment of estrogen receptor mediated diseases such as prostate cancer or benign prostate hyperplasia.

IT 787621-81-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

II

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-81-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-(trifluoromethyl)-, (2R,3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787621-88-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-ethyl-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN. 787621-99-2 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-fluoro-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (2R,3aR,4S,9bS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 787622-40-6 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 2-(difluoromethylene)-1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

RN 787622-43-9 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-78-0 CAPLUS

CN Cyclopenta[c][1]benzopyran-8-ol, 1,2,3,3a,4,9b-hexahydro-4-(4-hydroxyphenyl)-2-[(trimethylsilyl)ethynyl]-, (3aS,4R,9bR)- (9CI) (CA INDEX NAME)

## IT 787622-29-1P 787622-41-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopenta[c]chromenols as selective estrogen receptor-beta agonists)

RN 787622-29-1 CAPLUS

CN Cyclopenta[c][1]benzopyran-2-ol, 1,2,3,3a,4,9b-hexahydro-8-(phenylmethoxy)-4-[4-(phenylmethoxy)phenyl]-, (2R,3aR,4S,9bS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 787622-41-7 CAPLUS

CN Silane, (1,1-dimethylethyl) [4-[(3aR,4S,9bS)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,3a,4,9b-hexahydro-2[(trimethylsilyl)ethynyl]cyclopenta[c][1]benzopyran-4-yl]phenoxy]dimethyl, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$t-Bu$$
 $t-Bu$ 
 $t-Bu$ 
 $t-Bu$ 

PAGE 1-A

ye Me

L13 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2003:417738 CAPLUS Full-text

DOCUMENT NUMBER:

139:6768

TITLE:

Preparation of benzopyran derivatives as selective

estrogen receptor  $\beta$  agonists

INVENTOR(S):

Dodge, Jeffrey Alan; Krishnan, Venkatesh Gary; Lugar,

Charles Willis, III; Neubauer, Blake Lee; Norman,

Bryan Hurst; Pfeifer, Lance Allen; Richardson, Timothy

Ivo

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 138 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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							US 2002-363622P				
							EP 2002-793806	A3 20021107 <			

MARPAT 139:6768

GI

AB The title compds. I and II [wherein R1-R4 = independently H, alkyl, OH, alkoxy, halo, amido, or CF3; R5 = H or CF3; Y1-Y3 = independently H or alkyl; G = CH2, CH2CH2, or CH2CH2CH2] and stereoisomers, and pharmaceutical acceptable salts thereof are prepared as selective estrogen receptor  $\beta$ agonists for the treatment of prostate cancer. For example, the benzopyran III was prepared in a multi-step synthesis in moderate yield. III binds to estrogen receptor  $\beta$  (ER  $\beta$ ) with a Ki of <1 nM and Ki(ER  $\alpha$ )/Ki(ER  $\beta$ ) of 8.0. IT 533884-11-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug candidate; preparation of benzopyran derivs. as selective estrogen receptor  $\beta$  agonists)

RN533884-11-6 CAPLUS

CNPhenol, 4-[1,2,3,3a,4,9b-hexahydro-8-(trifluoromethyl)cyclopenta[c][1]benz opyran-4-yl]- (9CI) (CA INDEX NAME)

L13 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:689997 CAPLUS Full-text

DOCUMENT NUMBER: 130:38272

TITLE: A novel tandem bicyclization to form an indenopyran

ring system

AUTHOR(S): Chakraborty, Manisha; McConville, David B.; Saito,

Takeshi; Meng, Huihan; Rinaldi, Peter L.; Tessier,

Claire A.; Youngs, Wiley J.

CORPORATE SOURCE: Dep. of Chemistry, University of Akron, Akron, OH,

44325-3601, USA

SOURCE: Tetrahedron Letters (1998), 39(45),

8237-8340

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:38272

As a new palladium-copper catalyzed intramol. acetylene-zipper type bicyclization between alkyne and hydroxy functionality of an alkynyl hydroquinone has been observed to give a highly conjugated ring system.

IT 216777-12-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of indenopyrans by tandem bicyclization)

RN 216777-12-7 CAPLUS

CN 1,4-Benzenediol, 2-ethynyl-3-(1-ethynyl-2-hydroxy-3,4,8,9-tetramethylbenz[b]indeno[2,1-d]pyran-6-yl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1972:152831 CAPLUS Full-text

DOCUMENT NUMBER: 76:152831

TITLE: Condensation of phenyl ethynyl ketone with

cyclopentadiene. Reinvestigation

AUTHOR(S): Venkataramani, P. S.; Chandrasekharan, S.;

Swaminathan, S.

CORPORATE SOURCE: Dep. Org. Chem., Univ. Madras, Madras, India

SOURCE: Tetrahedron (1972), 28(5), 1249-55

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

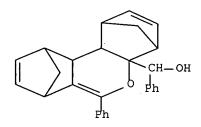
AΒ The earlier structural assignment of 2-benzoylnorborna-diene (I) for the product obtained by the condensation of PhC-(O)C.tplbond.CH with cyclopentadiene is now revised to a dimeric structure, II.

IT 36144-49-7P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 36144-49-7 CAPLUS

CN 1,4:7,10-Dimethano-4aH-dibenzo[b,d]pyran-4a-methanol, 1,4,7,10,10a,10bhexahydro- $\alpha$ , 6-diphenyl-,  $[1\alpha, 4\alpha, 4a\beta(R^*), 7\beta, 10]$ . beta.,  $10a\alpha$ ,  $10b\beta$ ] - (9CI) (CA INDEX NAME)



L13 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1969:77707 CAPLUS Full-text

DOCUMENT NUMBER: TITLE:

SOURCE:

70:77707 Experiments in the brazilane series. I.

Preparation

of 2-phenyl-5',6',7-trimethoxybrazilane

AUTHOR (S):

Morsingh, Francis

CORPORATE SOURCE:

Univ. Malaya, Kuala Lumpur, Malay. Tetrahedron (1969), 25(2), 355-9

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

LANGUAGE:

Journal English

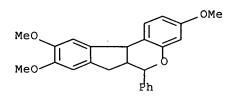
AB Superposition of flavan on brazilane would afford 2-phenylbrazilane. Although this structure has not yet been isolated, biogenetically it is feasible. The synthesis of 2-phenyl-5',6',7-trimethoxybrazilane is described.

IT 21834-73-1P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

21834-73-1 CAPLUS RN

Benz[b]indeno[1,2-d]pyran, 6,6a,7,11b-tetrahydro-3,9,10-trimethoxy-6-CN phenyl- (8CI) (CA INDEX NAME)



L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1946:23981 CAPLUS Full-text

DOCUMENT NUMBER:

40:23981

ORIGINAL REFERENCE NO.: 40:4709e-i,4710a-b

TITLE: Condensation of tetraphenylbutynediol with phenol

AUTHOR(S): Zal'kind, Yu. S.; Teterin, V. K.; Kuznetsov, S. G.

CORPORATE SOURCE: Leningrad Chem. Tech. Inst.

SOURCE: Zhurnal Obshchei Khimii (1945), 15, 488-98

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal LANGUAGE: English

AΒ [.tplbond.CC(OH)Ph2]2 (I) (30 g.), 87.6 g. PhOH, 60 cc. benzene and 0.4 q. dry H2NC6H4SO3H were refluxed for 2 h. with continuous removal of water by means of a Stark-Dean type collector, in which 3.35 cc. H2O was collected at the end of the reaction; after cooling and dilution with benzene, the crystalline and the liquid portions were steam-distilled to remove the solvent. There were obtained 28.7 g. crystalline matter and 16.7 g. red resin. Prolonged recrystn. from benzene, CHCl3, and ligroin gave the following products: 21.5 g. 1diphenylmethylene-2-p-hydroxyphenyl-3-phenylindene, m. 255° (II), yelloworange needles; 2.8 g. 1-diphenylmethylene-2- phenoxy-3-phenylindene (III), m. 223°, orange prisms; 1.2 g. 2,2,5,5-tetraphenyl-3-phenoxy-2,5-dihydrofuran, m. 176°, colorless needles; and 0.4 g. 2,2,3'-triphenyl-1',2',3,4-indenochroman (IV), m. 216-17°, colorless parallelopipeds. II was converted into the MeO derivative, m. 176-7°, by boiling with MeI in the presence of K2CO3 in Me2CO. or by treatment with Me2SO4 in 20% NaOH; rapid crystallization from Me2CO leads to yellow needles of the above m.p., slow crystallization gives large red-brown parallelopipeds, m. 167-8°. III was prepared by an alternate method for identification: 10.5 g. I in 150 cc. Et20 was treated with 22.5 g. PCl3 at 1°over 5 h., stirred for 2 h. at 0° and for 4 h. at room temperature to yield, after removal of the solvent, hydrolysis, and crystallization from ligroin 1.0 g. 1-diphenylmethylene-2-chloro-3- phenylindene, m. 157° (cf. Wieland and Kloss, C.A. 23, 3696), and 3 unidentified products m. 147-8° (4.5 g.), m. 194-5° (0.2 g.), and m. 165° (0.4 g.); 0.4 g. of the chloride was added to a solution of 0.1 g. K in 2 g. molten PhOH and heated slowly to 220° for 1 h.; after treatment with alkaline water, extraction of the precipitate with EtOH, and crystallization of the residue from benzene-petr. ether there was obtained a product identical with III, m. 223°, above. Boiling of this in MePh in the presence of sulfanilic acid failed to effect any isomerization. IV on boiling with alc. KOH is transformed into 2 substances which were unidentified: colorless, m. 230° (from EtOH, then EtOHMe2CO), and orange, m. 208-19°, with the former transforming into a product m. 208-14°, on heating above the m.p. The condensation of I with PhOH was also conducted in the presence of the following catalysts: activated Chasoviarskii clay, H2SO4-AcOH, and glacial The 1st catalyst gave results similar to sulfanilic acid while the 2nd catalyst gave only II, m. 255°, in 98% yield (crude); the 3rd catalyst gave only a resinous, ill-defined mixture of some transformation products of the glycol without condensation with PhOH.

IT 860186-11-4P, Benz[b] indeno[2,1-d] pyran, 6,6a-dihydro-6,6,11triphenyl-

RL: PREP (Preparation)

(preparation of)

RN 860186-11-4 CAPLUS

CN Benz[b]indeno[2,1-d]pyran, 6,6a-dihydro-6,6,11-triphenyl- (4CI) (CA INDEX NAME)

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